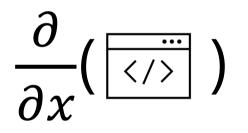
PROBABILISTIC AND DIFFERENTIABLE PROGRAMMING

V7: Automatic Differentiation (AD)

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Today's Agenda

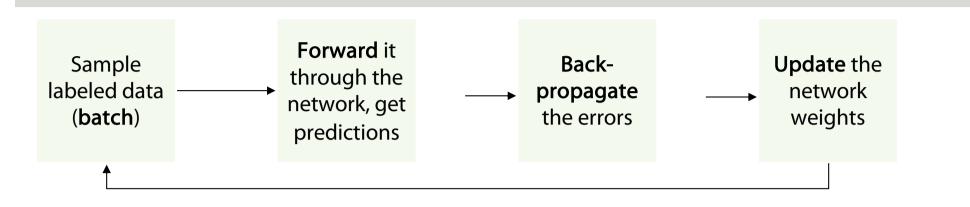




WHY YOU NEED AD

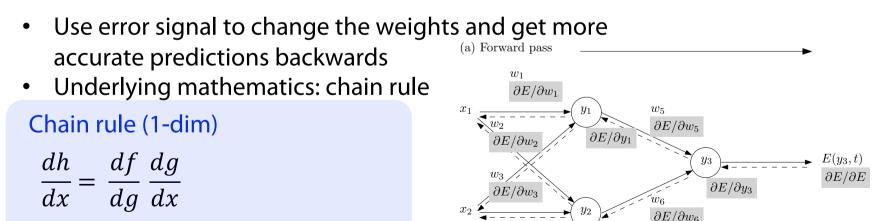


Reminder: Backprop = AD in reverse mode



Backpropagation idea

 Generate error signal that measures difference between predictions and target values



 w_{4}

 $\partial E / \partial w_4$

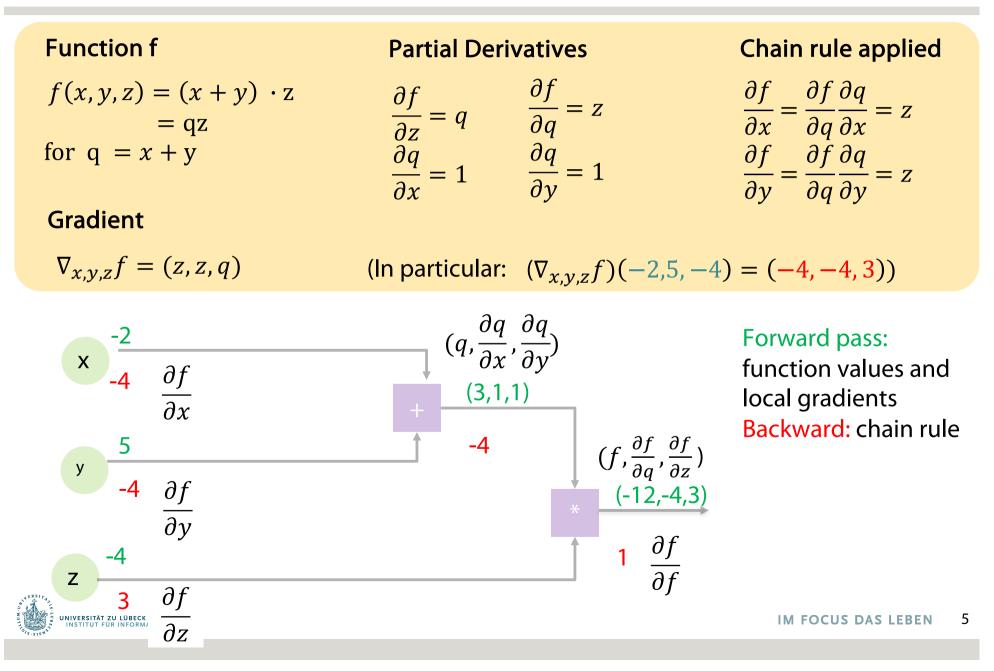
 $\partial E/\partial y_2$

$$(for h(x) = f(g(x)))$$



(b) Backward pass

Reminder: Computational graph perspective



- To solve optimisation problems using gradient methods we need to compute the gradients (derivatives) of the objective with respect to the parameters.
 - In neural nets we're talking about the gradients of the loss function, L with respect to the parameters θ
 - AD is at the heart of "Differentiable Programming" (the next big thing after deep learning)
 - AD is a topic on its own
 - But has been come into focus with Differentiable Programming and lead to many developments in the intersection of programming languages, numerical computing, and ML



- Symbolically differentiate the function with respect to its parameters
 - by hand
 - using a CAS
- Make estimates using finite differences

$$f'(a) \approx \frac{f(a+he_i)-f(a)}{h}$$

 Problem: Static, expression swell. Can't differentiate algorithms

 Problem: Numerical errors (such as rounding and truncation errors)



Problem with symbolic computation

$$\frac{d(f(x) \cdot g(x))}{dx} = \frac{d f(x)}{dx} g(x) + \frac{d g(x)}{dx} f(x) \quad \text{(Product rule)}$$
$$- h(x) := g(x) \cdot f(x)$$

- $-\frac{dh(x)}{dx}$ and *h* have two components in common
- This may also be the case for f.

 $\mathcal{G}(\mathcal{O})$

- Symbollically calculating f won't profit from common parts of f and $\frac{df(x)}{dx}$



Problems with numerical calculation

Truncation error: Approximation error due to not sufficiently small *h*

- tends to 0 for $h \rightarrow 0$

Can be mitigated partly by using centered approximation

$$f'(a) \approx \frac{f(a+he_i)-f(a-he_i)}{h}$$

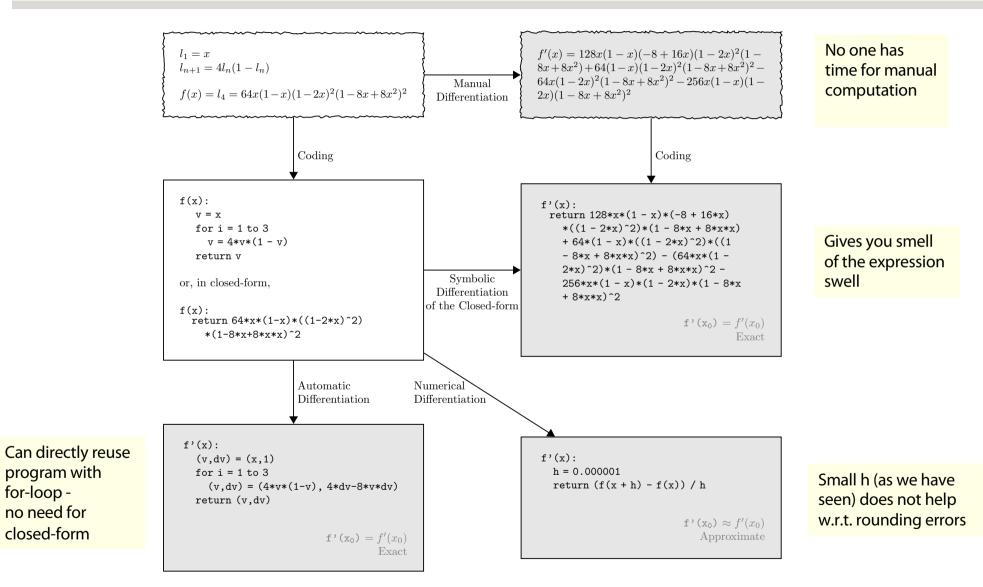
(error shift from O(h) to $O(h^2)$)

UNIVERSITÄT ZU LÜBECK INSTITUT FÜR INFORMATIONSSYSTEM Rounding error: due to limited precision in computation

- Increases for
$$h \rightarrow 0$$

- Automatic Differentiation is a method to get exact derivatives efficiently, by storing information as you go forward that you can reuse as you go backwards.
 - Takes code that computes a function and uses that to compute the derivative of that function.
 - The goal isn't to obtain closed-form solutions, but to be able to write a program that efficiently computes the derivatives.







Ex: Baydin et al. 2017

AUTOMATIZATION



From Differentiation to Programming

• Example (Math) x = ? y = ? a = xy $b = \sin(x)$ z = a + b• Example (code) x = ? Y = ? a = x * y $b = \sin(x)$ z = a + b



The chain rule for vectors

Given functions f, g with

 $- \mathbb{R}^m \xrightarrow{g} \mathbb{R}^n \xrightarrow{f} \mathbb{R}$

$$-x \mapsto y = g(x) \mapsto z = f(y)$$

the chain rule leads to the partial derivatives

$$\frac{\partial z}{\partial x_i} = \sum_j \frac{\partial z}{\partial y_j} \frac{\partial y_j}{\partial x_i}$$

(in short form: $\nabla_x z = \left(\frac{\partial y}{\partial x}\right)^\top \nabla_y z$
where $\left(\frac{\partial y}{\partial x}\right)$ is the *n x m* Jacobian matrix of *g*



Let us rename for the following

Given functions f, g with

 $- \mathbb{R}^m \xrightarrow{g} \mathbb{R}^n \xrightarrow{f} \mathbb{R}$

$$-t \mapsto u = g(x) \mapsto w = f(u)$$

the chain rule leads to the partial derivatives

$$\frac{\partial w}{\partial t} = \sum_{j} \frac{\partial w}{\partial u_{j}} \frac{\partial u_{j}}{\partial t}$$

w is some output variable from a family of outputs $\{w_i\}$ and u_i are the inputs variables *w* depends on.



Applying the chain rule

Example expression x = ? y = ? a = xy b = sin(x) z = a + b	Derivatives w.r.t. some yet to be given variable t $\frac{\partial x}{\partial t} = ?$ $\frac{\partial y}{\partial t} = ?$ $\frac{\partial a}{\partial t} = x \frac{\partial y}{\partial t} + y \frac{\partial x}{\partial t}$ $\frac{\partial b}{\partial t} = \cos x \frac{\partial x}{\partial t}$ $\frac{\partial b}{\partial t} = \cos x \frac{\partial x}{\partial t}$ $\frac{\partial z}{\partial t} = \frac{\partial a}{\partial t} + \frac{\partial b}{\partial t}$	
• If we substitute $t = x$ we get an algorithm for computing $\frac{\partial z}{\partial x}$. • Choosing $t = y$ similarly gives $\frac{\partial z}{\partial y}$.		



Translating to code

Derivatives as programs

Substituting t = x

$$dx = 1$$

$$dy = 0$$

$$da = y * dx + x * dy$$

$$db = cos(x)*dx$$

$$dz = da + db$$

(Using the notation

$$d\mathbf{x} = \frac{\partial x}{\partial t}, d\mathbf{y} = \frac{\partial y}{\partial t}, \dots$$
)

So, to compute $\frac{\partial z}{\partial x}$ just seed algorithm with dx = 1, dy = 0



Translating to code

Substituting t = y dx = 0 dy = 1 da = y * dx + x * dy db = cos(x)*dxdz = da + db

(Using the notation

$$d\mathbf{x} = \frac{\partial x}{\partial t}, d\mathbf{y} = \frac{\partial y}{\partial t}, \dots$$
)

So, to compute $\frac{\partial z}{\partial y}$ just seed algorithm with dx = 0, dy = 1



Making Rules

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- Idea of the examples can be generalized to arbitrary functions
- Need to describe rules for translation program evaluating expression => program evaluating derivates
- These are just rules known from mathematics for calculating derivates, e.g.

-c = a + b	=>	dc = da + db
- c = a * b	=>	dc = b * da + a * db
-c = sin(a)	=>	dc = cos(a) * da

Note: These rules are used on number-level (not for symbolic computation of derivatives)

Further Rules

 $c = a - b \qquad => \qquad dc = da - db$ $c = a / b \qquad => \qquad dc = da/b - a*db/b**2$ $c = a**b \qquad => \qquad dc = b*a**(b-1)*da + log(a)*a**b*db$ $c = cos(a) \qquad => \qquad dc = -sin(a) * da$ $c = tan(a) \qquad => \qquad dc = da/cos(a)**2$

 $(a^{**b} \text{ stands for } a^b)$



FORWARD MODE



Forward Mode AD

- To translate using the rules we simply replace each primitive operation in the original program by its differential analogue.
- The order of computation remains unchanged: if a statement *K* is evaluated before another statement *L*, then the differential analogue of *K* is evaluated before the analogue statement of *L*.
- This is Forward-mode Automatic Differentiation.
 - Nice feature: Interleaving (function evaluation and derivatives) is possible
 - Bad feature: Need to rerun program to compute derivative for each input (in particular for gradient)



Interleave computing expression and derivatives

$$x = ?
dx = ?
y = ?
dy = ?
a = x * y
da = y * dx + x * dy
b = sin(x)
db = cos(x)*dx
z = a + b
dz = da + db$$

- Can keep track of value and gradient at the same time
- Can be mathematically founded using "dual numbers"
- Leads to direct simple implementation of AD



The Jacobian in Forward Mode AD

- $f: \mathbb{R}^n \to \mathbb{R}^m; \mathbf{x} \mapsto \mathbf{z}$
- Calculate derivatives
 w.r.t. ith variable x_i for all outputs z_i in one pass

$$\frac{\partial z}{\partial x} = \begin{pmatrix} \frac{\partial z_1}{\partial x_1}(a) & \cdots \frac{\partial z_1}{\partial x_i}(a) & \frac{\partial z_1}{\partial x_n}(a) \\ \vdots & \ddots & \vdots \\ \frac{\partial z_m}{\partial x_1}(a) & \cdots \frac{\partial z_m}{\partial x_i}(a) & \cdots & \frac{\partial z_m}{\partial x_n}(a) \end{pmatrix}$$

- Efficient calculating product w.r.t. vector *r*
 - $-\frac{\partial z}{\partial x}\cdot r$

$$dx_1 = r_1, ..., dx_n = r_n$$

• Special case f: $\mathbb{R}^n \to \mathbb{R}$; $x \mapsto z$

Calculate directional derivate in direction *r*.

$$-\nabla f \cdot r$$



Another view on AD

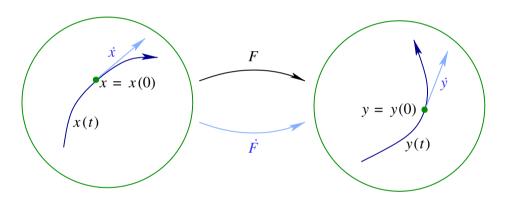
- $f: \mathbb{R}^n \to \mathbb{R}^m$
 - $-v_{i-n} = x_i$, i = 1, ..., n input variables
 - v_i , i = 1, ..., l intermediate variables
 - $y_{m-i} = v_{l-i}$, i = m 1, ..., 0 output variables
 - $v_i = \phi_i (v_j)_{j < i}$, $\phi_i : \mathbb{R}^{n_j} \to \mathbb{R}$ (elemental functions)
 - where ≺ is precedence relation (*j* ≺ *i* iff *v*_*i* directly depends on *v*_*j*)
 - n_j number of elements preceding v_j

$$- u_i = (v_j)_{j \prec i}$$



Forward mode AD = Tangents mapping

- Assume you have time-depending paths x(t), y(t)
- Forward mode AD is mapping function evaluation (F: $x \mapsto y$) plus tangents mapping $\dot{F}: \dot{x} \mapsto \dot{y}$



$$\begin{bmatrix} v_{i-n}, \dot{v}_{i-n} \end{bmatrix} = \begin{bmatrix} x_i, \dot{x}_i \end{bmatrix} & \text{for } i = 1, \dots, n \\ \begin{bmatrix} v_i, \dot{v}_i \end{bmatrix} = \begin{bmatrix} \phi_i(u_i), \dot{\phi}_i(u_i, \dot{u}_i) \end{bmatrix} & \text{for } i = 1, \dots, l \\ \begin{bmatrix} y_{m-i}, \dot{y}_{m-i} \end{bmatrix} = \begin{bmatrix} v_{l-i}, \dot{v}_{l-i} \end{bmatrix} & \text{for } i = 0, \dots, m -$$



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Dual numbers (Clifford 1873)

- Want to mathematize parallel evaluation of f, f'
- Dual numbers have the form $(v + \dot{v}\epsilon)$ where
 - $v, \dot{v} \in \mathbb{R}$
 - ϵ is a nilpotent element ($\epsilon^2 = 0, \epsilon \neq 0$)
 - compare with complex numbers x + yi where $i^2 = -1$, which can be considered as pairs in \mathbb{R}^2 (more general: quaterions)
- Gives intended behaviour mirroring symbolic derivation
 - $-(v + \dot{v}\epsilon) + (u + \dot{u}\epsilon) = (v + u) + (\dot{v} + \dot{u})\epsilon$
 - $(v + \dot{v}\epsilon)(u + \dot{u}\epsilon) = (vu) + (v\dot{u} + \dot{v}u)\epsilon$



Dual numbers (Clifford 1873)

• Can define functions f on dual numbers by $f(v + \dot{v}\epsilon) = f(v) + f'(v)\dot{v}\epsilon$ (results from Taylor series application)

(results from Taylor series application)

- Then: Chain rule works as expected: $f(g(v + \dot{v}\epsilon)) = f(g(v) + g'(v)\dot{v}\epsilon)$ $= f(g(v)) + f'(g(v))g'(v)\dot{v}\epsilon)$
- Can extract derivative

 $\frac{df}{dx}(v) = \epsilon - coeff(dual - version(f)(v + 1\epsilon))$



REVERSE MODE



Reverse Mode AD

- Whilst Forward-mode AD is easy to implement, it comes with a very big disadvantage...
- For every variable we wish to compute the gradient with respect to, we have to run the *complete program* again.
- This is obviously going to be a problem if we're talking about the gradients of a function with very many parameters (e.g. a deep network).
- A solution is Reverse Mode Automatic Differentiation.



Reversing the Chain Rule

- Conceptually, chain rule doesn't care about role of enumerator and denominator – can turn it upside down
 - $-\frac{\partial w}{\partial t}$ becomes
 - $-\frac{\partial t}{\partial w}$ becomes by renaming (s for t and u for w)
 - $-\frac{\partial s}{\partial u}$ is by applying chain

$$-\frac{\partial s}{\partial u} = \sum_{j} \frac{\partial w_i}{\partial u} \frac{\partial s}{\partial w_i}$$

- *u* is some input variable
- w_i s are output variables depending on u
- *s* is the yet-to-be-given variable

Now can compute in 1-pass in parallel: $\frac{\partial s}{\partial x}$, $\frac{\partial s}{\partial y}$, ...

Example

$$\frac{\partial s}{\partial u} = \sum_{j} \frac{\partial w_{i}}{\partial u} \frac{\partial s}{\partial w_{i}}$$

$$x = ?$$

$$y = ?$$

$$a = xy$$

$$b = \sin(x)$$

$$z = a + b$$

$$\frac{\partial s}{\partial u} = ?$$

$$\frac{\partial s}{\partial b} = \frac{\partial z}{\partial b} \frac{\partial s}{\partial z} = \frac{\partial s}{\partial z}$$

$$\frac{\partial s}{\partial a} = \frac{\partial z}{\partial a} \frac{\partial s}{\partial z} = \frac{\partial s}{\partial z}$$

$$\frac{\partial s}{\partial a} = \frac{\partial z}{\partial a} \frac{\partial s}{\partial z} = \frac{\partial s}{\partial z}$$

$$\frac{\partial s}{\partial y} = \frac{\partial a}{\partial y} \frac{\partial s}{\partial a} = x \frac{\partial s}{\partial a}$$

$$\frac{\partial s}{\partial y} = \frac{\partial a}{\partial x} \frac{\partial s}{\partial a} + \frac{\partial b}{\partial x} \frac{\partial s}{\partial b}$$

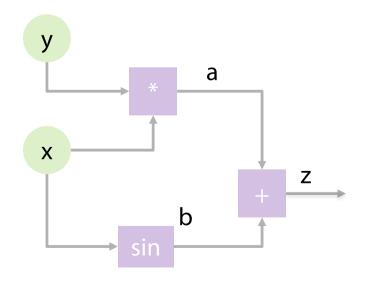
$$= y \frac{\partial s}{\partial a} + \cos x \frac{\partial s}{\partial b}$$

$$= (y + \cos x) \frac{\partial s}{\partial z}$$



Visualising dependencies

- Differentiating in reverse can be quite mind-bending: instead of asking what input variables an output depends on, we have to ask what output variables a given input variable can affect.
- We can see this visually by drawing a dependency graph of the expression (e.g. x effects a and b):





Translating to Code

- As before we replace the derivatives (∂s/∂z, ∂s/ ∂b,...) with variables (gz, gb, ...) which we call adjoint variables:
 - -gz = ? -gb = gz We need only 1 pass for Calculating all derivatives
 - -ga = gz

-gy = x * ga

$$-gx = y * ga + cos(x) * gb$$

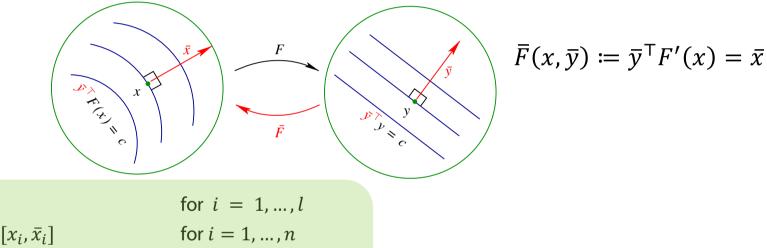
• Substituting s = z in equations gives both gradients $\frac{\partial z}{\partial x}$

and
$$\frac{\partial z}{\partial y}$$
 in last two lines



Reverse mode AD = Co-tangents mapping

• Reverse mode AD: function evaluation, F: $x \mapsto y$, plus co-tangents mapping by adjoint $\overline{F}: \overline{y} \mapsto \overline{x}$



$v_i = 0$	for $i = 1, \dots, l$	
$[v_{i-n}, \bar{v}_{i-1}] = [x_i, \bar{x}_i]$ Push(v_i)	for $i = 1,, n$	
$v_i = \phi_i(u_i)$	for $i = 1, \dots, l$	
$y_{m-1} = v_{l-1}$	for $i = 0,, m - 1$	
$ \bar{v}_{l-i} = \bar{y}_{m-1} $ $ v_i \leftarrow pop() $	for $i = 0,, m - 1$	(simple algorithm
$\bar{u}_i + = \bar{v}_i * \nabla \phi_i(u_i)$	for <i>l</i> , , 1	without sophisticated memory management:
$ \begin{array}{l} \nu_i = 0\\ \bar{x}_i = \bar{\nu}_{i-n} \end{array} $	for $i = 1,, n$	just using stack)

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But wait... Limitations of Reverse Mode AD

- We have a problem dual to that of forward AD: Now have to run the program for each outvariable one is interested in differentiating
- Example
 - $-z = 2x + \sin x$
 - $-v = 4x + \cos x$

Calculating $\frac{\partial z}{\partial x}$ and $\frac{\partial v}{\partial x}$ each requires running the programm

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- Cannot interleave the calculations as they appear to be in reverse mode.=> Recent research on automatization
- So: Reverse AD has advantage only if number of output variables much smaller than number of input variables FOCUS DAS LEBEN

Implementing Reverse Mode AD

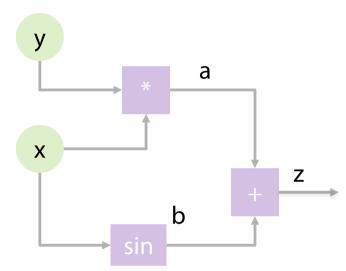
There are two ways to implement Reverse AD:

- 1. We can parse the original program and generate the *adjoint* program that calculates the derivatives.
 - Potentially hard to do.
 - Static, so can only be used to differentiate algorithms that have parameters predefined.
 - But, efficient (lots of opportunities for optimisation)
- 2. We can make a *dynamic* implementation by constructing a graph that represents the original expression as the program runs.



Constructing an expression graph (in Python)

• Goal: get a graph as



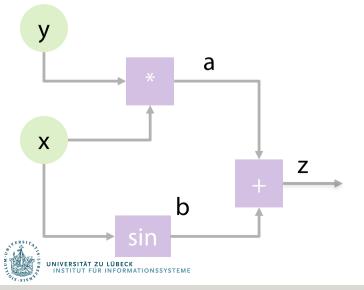
- Root of the graph are independent variables x, y
- Can have children (initially empty): nodes that depending on parent

$$y = Var (4.2)$$



Building expressions

- Expression creation
- Self-registration of each expression *u* as a child of each of its dependencies *w_i*
- Also register weight $\frac{\partial w_i}{\partial u}$ (used for gradient calculation)



class Var:

```
def __mul__(self, other):
   z = Var(self.value * other.value)
```

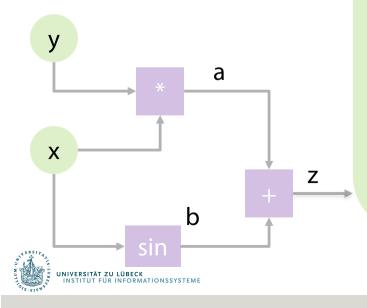
weight = dz/dself = other.value
self.children.append((other.value, z))

weight = dz/dother = self.value
other.children.append((self.value, z))
return z

"a" is a new Var that is a child of both x and y # a=x*y

Computing gradients

- Propagate
 Derivatives
- Cache derivatives in grad_value



```
class Var:
def __init__(self):
...
self.grad_value = None
def grad(self):
    if self.grad_value is None:
    # using chain rule
    self.grad_value =
        sum(weight * var.grad()
            for weight, var in self.children)
return self.grad_value ...
```

```
a.grad_value = 1.0
print("da/dx_=_{}".format(x.grad()))
```

Optimising reverse Mode AD

- The outline implemntation not very space efficient
 - Instead of children directly store in indices (Wengert list, tape)
- Space efficiency for reverse AD is challenging hence research topic
 - Count-Trailing-Zeros CTZ): trade-off computation for memory of caches (Griewank 92).
 - But, in reality memory is relatively cheap (if managed well)



CTZ example

- Idea: Hierarchical cache storing only $O(\log(N))$ of all N values in expression in forward sweep and maintained during reverse sweep
 - Cache₀ store first value
 - Cache₁ stores value at $\frac{1}{2}$ down chain
 - Cache₂ stores value at ³/₄ down the chain ...
 - Cache_{n-1} stores value at n/n+1 down the chain
- Assume linear expression of N= 16 Operators
 - 0123456789abcdef (value indices)
 - X-----X----X----X (stored value indication)



CTZ example (continued)

- Reverse sweep (with head postion)
 - 0123456789abcdef (can swee over e,f)

– X-----X----XXX

- 0123456789abcdef (d not cached, recalculate) – X-----X----XXX

- 0123456789abcdef – X-----X----X X +-X

(d not cached, recalculate) from cached c)



CTZ example (continued)

Reverse sweep (with head postion _) •

+-X

- 0123456789abcdef (sweep over c, missing b,
- X-----X----X = sweep to 8 and cache a)

(recompute 9 from 8, then 7to be recomputed

move to 0, store along 6,4)

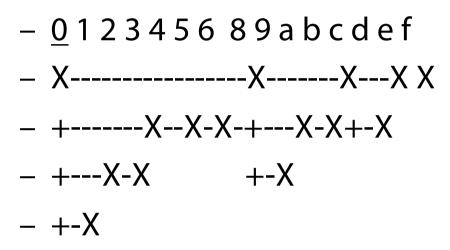
+-X

(and so on ...)



CTZ example (continued)

• In the end





Uhhh, a lecture with a hopefully useful

APPENDIX



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Color Convention in this Course

- Formulae, when occurring inline
- Newly introduced terminology and definitions
- Important results (observations, theorems) as well as emphasizing some aspects
- Examples are given with standard orange with possibly light orange frame
- Comments and notes in nearly opaque post-it
- Algorithms and program code
- Reminders (in the grey fog of your memory)



Today's lecture is based on the following

- Jonathon Hare: Lecture 5 of course "COMP6248 Differentiable Programming (and some Deep Learning)" <u>http://comp6248.ecs.soton.ac.uk/</u>
- Blog post by Rufflewind: Reverse-mode automatic differentiation: a tutorial <u>https://rufflewind.com/2016-12-30/reverse-mode-automatic-differentiation</u>
- A. G. Baydin, B. A. Pearlmutter, A. A. Radul, and J. M. Siskind. Automatic differentiation in machine learning: A survey. J. Mach. Learn. Res., 18(1):5595–5637, Jan. 2017.
- A. H. Gebremedhin and A. Walther. An introduction to algorithmic differentiation. WIREs Data Mining and Knowledge Discovery, 10(1):e1334, 2020.



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- A. Griewank. Achieving logarithmic growth of temporal and spatial complexity in reverse automatic differentiation. Optimization Methods and Software, 1(1):35–54, 1992.

